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A. Fast Two-dimensional Model

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C. Research Objectives

The objective of this research is to use a two-dimensional (altitude and latitude) model of the atmosphere to investigate problems relating to the variability of the dynamics and temperature of the atmosphere on the ozone distribution, solar cycle variations of atmospheric constituents, the sensitivity of model results to tropospheric trace gas sources, and assessment computations of changes in ozone related to manmade influences.

D. Progress and Results

We have contrasted two-dimensional (2D) model results in which the odd nitrogen family was transported together with model results in which the odd nitrogen species were transported separately and found that family approximations are adequate for perturbation scenario calculations. However, because HNO_3 data are available for comparison with calculated values and family approximations are poor for HNO_3 during winter, in future model simulations HNO_3 will be transported separately.

The sensitivity of ozone and ozone perturbation scenarios due to dynamical inputs were investigated and it was found that although total ozone was extremely sensitive to the circulation between 1000 and 100 mbar, the perturbation scenarios were relatively insensitive to the dynamical inputs.

The effect of solar proton events (SPEs) on the middle atmosphere during the two solar cycle period from 1963-85 was investigated and it was found that: 1) odd nitrogen does not build up over solar cycle periods but decreases to ambient values in 2-6 months following even a major SPE and 2) only the August 1972 SPE caused significant stratospheric ozone depletion at high latitudes.

All eight assessment scenarios of interest were investigated for the United Nations Environmental Program "Scientific Assessment of Stratospheric Ozone:1989" with the use of our 2D model.

We took part in an international 2D model intercomparison held at Virginia Beach, VA in September 1988 and have been actively involved in the conference proceedings which will be published in August 1989 concerning that meeting.

We cooperate with the three-dimensional (3D) modeling effort at NASA/GSFC (Code 616) and provide initial conditions from our 2D model for use in the 3D model.

E. Journal Publications

Douglass, A. R., C. H. Jackman, and R. S. Stolarski, Comparison of model results transporting the odd nitrogen family with results transporting separate odd nitrogen species, J. Geophys. Res., 94, 9862-9872, 1989.

Jackman, C. H., A. R. Douglass, P. D. Guthrie, and R. S. Stolarski, The sensitivity of total ozone and ozone perturbation scenarios in a two-dimensional model due to dynamical inputs, J. Geophys. Res., 94, 9873-9887, 1989.

Jackman, C. H., A. R. Douglass, and P. E. Meade, The effects of solar particle events on the middle atmosphere, in press, Middle Atmosphere Handbook, 1989.

Jackman, C. H., A. R. Douglass, P. A. Newman, and P. D. Guthrie, Effect of computed horizontal diffusion coefficients on two-dimensional assessment studies, in press, Proceedings of the Quadrennial Ozone Symposium held at Gottingen, West Germany, August 8-13, 1988.

Douglass, A. R., C. H. Jackman, and R. S. Stolarski, Two-dimensional model comparisons of odd nitrogen family chemistry with separate calculations for the odd nitrogen species, in press, Proceedings of the Quadrennial Ozone Symposium held at Gottingen, West Germany, August 8-13, 1988.

UATDAP Research Summary 1988-1989

A. Title of Research Task

Modeling of Chemistry and Transport in a Two-Dimensional Model of the Terrestrial Stratosphere and Mesosphere

B. Investigations and Institutions

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C. Abstract of Research Objectives

The focus of our research program is the achievement of a quantitative understanding of the spatial distribution and temporal variation of chemical species in the terrestrial middle atmosphere, with emphasis on ozone. Although not directed at assessments of anthropogenic impacts, our activities contribute to a refinement of model descriptions of chemical and dynamical processes that are needed for assessment tasks.

D. Summary of Progress and Results

1. One week (May 1-7, 1979) of data from the Nimbus 7 Limb Infrared Monitor of the Stratosphere (LIMS) was analyzed in detail, with emphasis on the ozone abundance and its temperature sensitivity between 0.1 and 6 mbar, covering the upper stratosphere and lower mesosphere. The zonally averaged ozone profile (30°-35°N latitude) is compared with results from a simplified photochemical model that assumes ozone to be in photochemical steady state. The model ozone profile is systematically lower than the observed profile. Changes in O_2 photolysis and O_3 formation could eliminate most of the differences in the whole altitude range. Thus one does not have to invoke one or more missing key reactions in current photochemical models in order to explain this systematic discrepancy. The LIMS-derived values for the sensitivity of ozone to changes in temperature, θ_L, are compared with equilibrium model calculations, θ_E, which include the temperature-driven opacity feedback effect on photodissociation rate constants. Given the noise of the data, there is fair agreement in the mesosphere, but below 1 mbar, θ_L/θ_E decreases with increasing pressure. In the upper stratosphere the LIMS-derived θ values can be explained by a combination/superposition of waves with 1- to 5-day periods.

2. We examined the consequences of the eruption of the El Chichon volcano on the Earth's stratospheric chemistry. Formed after the eruption, the volcanic aerosol cloud, with a peak particle density at 27 km, was very efficient at altering the radiation field. A combination of this radiation change and the effect of a temperature variation of a few degrees causes the abundance of O_3 to decrease by 7% at 24 km, in good agreement with the SBUV measurements of a 5-10% decrease. A heterogeneous

reaction catalyzed by aerosol surfaces which transforms $ClNO_3$ into HCl provides a pathway for sequestering NO_x, and at the same time reduces $ClNO_3$ in favor of HCl. The inclusion of this reaction in the model leads to a satisfactory single-step explanation of the otherwise puzzling observations of significant decreases in NO and NO_2 and increases in HCl.

3. The gas-phase recombination of chlorine monoxide (ClO) has been investigated under the conditions of pressure and temperature that prevail in the Antarctic stratosphere during the period of maximum ozone (O_3) disappearance. Measured rate constants are less than one-half as great as the previously accepted values. One-dimensional model calculations based upon the new rate data indicate that currently accepted chemical mechanisms can quantitatively account for the observed O_3 losses in late spring 17 September to 7 October.

4. Extensive testing of the advective scheme, proposed by Prather (1986), has been carried out in support of the Caltech-JPL two-dimensional model of the middle atmosphere. Five types of numerical experiments including simple clock rotation and pure advection in 2-D have been investigated in detail. Upon comparing our numerical model results with analytic solutions, we find that the new algorithm can faithfully preserve concentration profiles and has essentially no numerical diffusion.

5. Using the Caltech-JPL two-dimensional transport model, with transport coefficients taken from Yang and Tung (1989), we have studied the time evolution of excess carbon 14 in the stratosphere and the troposphere from October, 1963 to December, 1966. The model provides a satisfactory simulation of the observed data. Due to the impulsive nature of its source, initial distributions of excess carbon 14 exhibit large spatial gradients. This permits important constraints on the range of diffusive transport coefficients in the lower stratosphere to be derived.

E. Journal Publications

Froidevaux, L., Allen, M., Berman, S., and Daughton, A. (1989). The mean ozone profile and its temperature sensitivity in the upper stratosphere and lower mesosphere: An analysis of LIMS observations. *J. Geophys. Res.* **94**, 6389-6417.

Michelangeli, D.V., Allen, M., and Yung, Y.L. (1989). El Chichon volcanic aerosols: Impact of radiative, thermal and chemical perturbations. *J. Geophys. Res.*, in press.

Shia, R.-L., Yung, Y.L., Allen, M., Zurek, R.W., and Crisp, D. (1989). Sensitivity study of advection and diffusion coefficients in a two-dimensional stratospheric model using excess carbon 14 data. *J. Geophys. Res.*, in press.

Sander, S.P., Friedl, R.R., and Yung, Y.L. (1989). ClO dimer in polar stratospheric chemistry: Rate of formation and implications for ozone loss. *Science*, in press.

Shia, R.-L., Ha, Y.L., Wen, J-S., and Yung, Y.L. (1989). Two-dimensional atmospheric transport and chemistry model: Numerical experiments with a new advection algorithm. *J. Geophys. Res.*, in press.

Biennial Research Summary

STRATOSPHERIC RADIATIVE PROCESSES AND THE 2-D CHEMICAL TRACER TRANSPORT CIRCULATION

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ABSTRACT

The distribution of O_3 and other trace gases is most strongly influenced by meridional transport at levels in the middle and lower stratosphere. GCM experiments show that the transport at these levels can be approximated by the diabatic circulation, which can be derived diagnostically from the net radiative heating rates. I am developing a hierarchy of fast, accurate methods for finding stratospheric net radiative heating rates. These heating rates will be used to specify the transport circulation in the Caltech 2-D Chemical Tracer Transport Model.

SUMMARY OF PROGRESS AND RESULTS

2-dimensional chemical tracer transport models are the best existing tools for studying the response of the stratosphere to observed changes in thermal structure and composition. The advective component of the meridional transport in these models is approximated by the diabatic circulation, which can be derived diagnostically from the net radiative heating rates. Accurate radiative transfer models are essential for this application because the net radiative heating rates are obtained by subtracting the almost-equal solar heating rates and thermal cooling rates at each stratospheric level. Small errors in the solar or thermal components can produce enormous errors in net heating rates and the strength of the derived diabatic circulation. This is particularly true at levels in the middle and lower stratosphere, where these components usually differ by less than 20%. I recently conducted an intercomparison of thermal cooling algorithms used by several 2-d groups, and found cooling rate errors twice this large. This result has serious implications for the validity of the 2-d modeling results derived by these groups. Our Quasi-Random Model rarely produces cooling rate errors larger than 5%, but requires much more computer time than those used by other groups. Faster radiative transfer algorithms are essential in 2-d chemical tracer transport models, because net radiative heating rates must be recomputed often as the atmospheric temperature and composition changes.

The Caltech radiative transfer model accounts for all important radiative processes at levels between the surface and 65 km. A Voigt Quasi-Random model is used to find the absorption by gases, and a delta-Eddington/Adding method is used to find fluxes and heating rates in absorbing, scattering atmospheres. This model agrees well with an accurate line-by-line model, but it requires much more computing time than the simpler models used by other 2-D modeling groups. We propose to address these problems by developing and implementing a new class of Correlated-k model. This model should provide the speed and accuracy needed in a broad range of stratospheric tracer transport modeling applications.

Upper Atmosphere Theory and Data Analysis (UATDAP) Program 1988-1989 Research Summary

A. Title of Research Task

MESOSPHERIC THEORY

B. Investigators and Institutions

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Collaborators
Y. Yung (Caltech), M. Allen and D. Crisp (JPL and Caltech)

(See the UATDAP Research Summary by Y. Yung et al., "Modeling of Chemistry and Transport with a Two-Dimensional Model of the Terrestrial Stratosphere and Mesosphere".)

C. Abstract of Research Objectives

This research task supports a collaborative effort between investigators at Caltech and JPL to understand quantitatively the structure and circulation of the upper atmosphere and the distribution there of photochemically or radiatively important trace constituents. This is done through numerical simulations of the observed tracer distributions, using one and two-dimensional models of coupled photochemical, dynamical and radiative processes.

D. Summary of Progress and Results

Extensive testing of the advective transport scheme proposed by Prather (1986) has been carried out in support of the Caltech-JPL two-dimensional model of the middle atmosphere. The implemented algorithm faithfully preserves concentration profiles and has essentially no numerical diffusion.

The Caltech-JPL two-dimensional transport model, with advective zonal-mean winds and eddy mixing coefficients taken from Yang and Tung (1989), has been used to simulate the time evolution of excess ^{14}C in the stratosphere and troposphere during 1963-1966. Due to the impulsive nature of its source, initial distributions of excess ^{14}C exhibit large spatial gradients. This permits important constraints to be derived on the range of the "effective" diffusive mixing in the lower stratosphere.

E. Journal Publications

Shia, R.-L., Y. L. Yung, M. Allen, R. W. Zurek and D. Crisp (1989). Sensitivity study of advection and diffusion coefficients in a two-dimensional stratospheric model using excess carbon 14 data. J. Geophys. Res., in press.

BIENNIAL RESEARCH SUMMARY

A. Dynamical Investigations of the Middle Atmosphere with a 2-D Model

B. Dr. Matthew H. Hitchman, Principal Investigator
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Dr. Guy Brasseur, Co-Investigator
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C. The fundamental goal is to improve our understanding of dynamics and tracer transport in the middle atmosphere through the use of a two dimensional numerical model. The model contains approximately 50 trace species, a detailed radiative code, and has fully interactive zonal mean and wave dynamics, including a new method of closure for the effects of planetary scale Rossby waves. Five areas of study are emphasized for the three year period 1 September 1988 - 31 August 1991: 1) a complete exploration of the impact of this new Rossby wave parameterization on the meridional circulation and tracer distributions, 2) transport at low latitudes, including the roles of photochemistry and wave driving in the semiannual and quasibiennial oscillations, 3) modeling the effects of heterogeneous processes on the ozone layer, and 4) systematically assessing the relative roles of annual insulation variation and wave driving by gravity, Rossby, and Kelvin waves in establishing the observed basic state.

D. Our grant began in September of 1988. 1) The main emphasis since that time has been in exploring the Rossby wave parameterization. We have performed many sensitivity studies and have diagnosed the feedbacks that result. In conjunction with Dr. Walter Robinson of the University of Illinois at Champagn-Urbana, we are comparing the WKBJ group velocity representation of Rossby wave activity propagation and absorption with a steady state linear wave model. There is general agreement and, where there are differences, the reasons are clear. 2) We have modified how winds are calculated in the model such that tropical winds have the capability to interact with gravity and Kelvin waves. We have recently added Kelvin waves to the model using the method of Plumb (1977). Initial results include a reasonable semiannual oscillation. 3) The model now has a threshold temperature below which polar stratospheric clouds are assumed to form and create additional odd chlorine. The parameterization has been tuned to yield spring ozone losses similar to what has been recently observed. Large uncertainties in the rates of microphysical processes limit the utility of this parameterization. 4) We have begun the fundamental study of causes of the basic state by calculating radiative equilibrium temperatures and exploring the differences that result from different basic assumptions regarding boundary conditions and allowed flows.

We have performed many model runs of perturbed trace gas scenarios in conjunction with the model intercomparison workshop held in Virginia Beach during September of 1988, and for the document "Scientific Assessment of Stratospheric Ozone: 1989", and have contributed sections and a summary of Chapter 3 for that document. The first publication below reflects work on understanding recent global ozone changes. The second describes the Rossby wave parameterization. The third documents our 2-D model in greater detail. In the fourth publication, the 2-D model was crucial in understanding the mechanism of how gravity wave driving causes the separated polar winter stratopause.

E. Publications

1) Brasseur, G., M. H. Hitchman, P. C. Simon, and A. De Rudder, 1988: Ozone reduction in the 1980's: A model simulation of anthropogenic and solar perturbations. *Geophys. Res. Lett.*, **15**, 1361-1364.

2) Hitchman, M. H. and G. Brasseur, 1988: Rossby wave activity in a two-dimensional model: Closure for wave driving and meridional eddy diffusivity. *J. Geophys. Res.*, **93**, 9405-9417.

3) Brasseur, G., M. H. Hitchman, S. Walters, M. Dymek, E. Falise, and M. Pirre, 1989: An interactive chemical dynamical radiative two-dimensional model of the middle atmosphere. *J. Geophys. Res.*, in press.

4) Hitchman, M. H., J. C. Gille, C. D. Rodgers, and G. Brasseur, 1989: The separated polar winter stratopause: A gravity wave driven climatological feature. *J. Atmos. Sci.*, **46**, 410-422.